

# Evaluation of 3013 Can Pressurization Due to H<sub>2</sub>O Radiolysis

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# Evaluation Parameters

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- Can Free Volume = 2126 ml
- Temperature = 50 °C
- Mass PuO<sub>2</sub> = 5000 g
  - 4410 g Pu-239, 590 g O
- Specific Surf Area = 1 m<sup>2</sup>/g
  - Total Surface Area = 5 x 10<sup>7</sup> cm<sup>2</sup>
- 2 wt. % H<sub>2</sub>O = 100 g = 5.56 moles
- P<sub>H<sub>2</sub>O, 2 wt. %, 50°c</sub> = nRT / V [if all H<sub>2</sub>O<sub>(a)</sub> converts to H<sub>2(g)</sub>]  
= 5.56 mol \* 1206 psi,ml / K,mol \* 323 K / 2162 ml = 1002 psi



# Kinetic Modeling Parameters

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- 2 wt. % H<sub>2</sub>O = 5.56 moles
- Total Surface Area =  $5 \times 10^7 \text{ cm}^2$
- Assume 10.5 Å<sup>2</sup> adsorption sites →  $1.58 \times 10^{-9} \text{ moles of sites / cm}^2$
- $1.58 \times 10^{-9} \text{ moles/cm}^2 * 5 \times 10^7 \text{ cm}^2 = 7.9 \times 10^{-2} \text{ moles per layer}$
- $5.56 \text{ moles} / 7.9 \times 10^{-2} \text{ moles per layer} \sim 70 \text{ layers of adsorbate}$
- Sufficient coverage of water to treat all layers equivalently



# Pressurization Mechanism

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RadCalc provides  $k_{\text{H}_2}$  as  $5 \times 10^{-9} \text{ sec}^{-1}$

$$k_{\text{O}_2} = 1.72 \times 10^3 * k_{\text{H}_2} = 8.6 \times 10^{-6}$$

(relation derived from evaluation of Ron Livingston's data sets at 1-2 wt. % H<sub>2</sub>O).



# Water Reformation

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What is  $k_R$  ?

$k_R$  is most likely highly dependent on water coverage

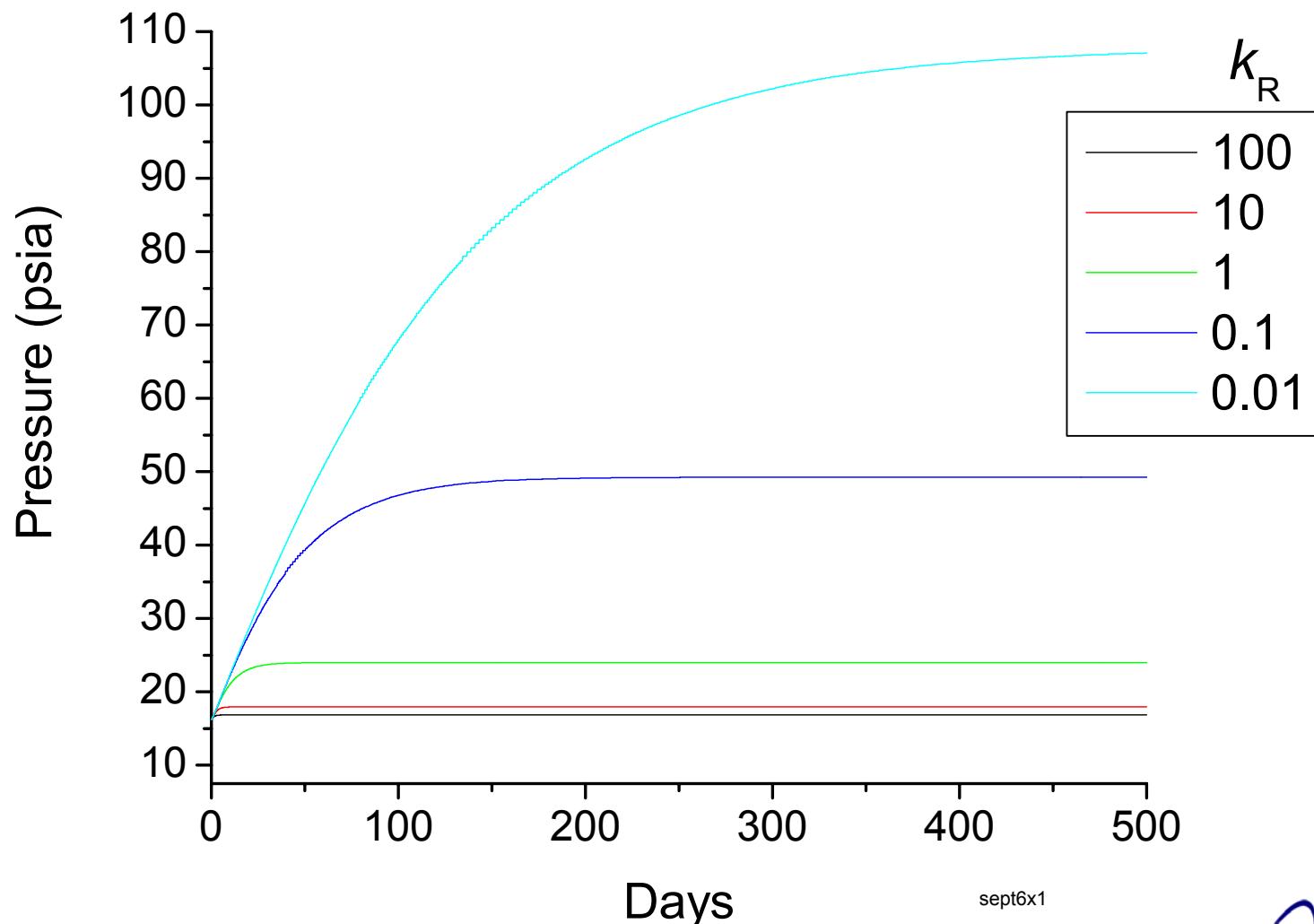
Evaluation of Ron Livingston's data indicates that:

$k_R \sim 10^{-2}$  at 2 wt. % water

$k_R \sim 10^2$  at 1 wt. % water



# Can Pressure

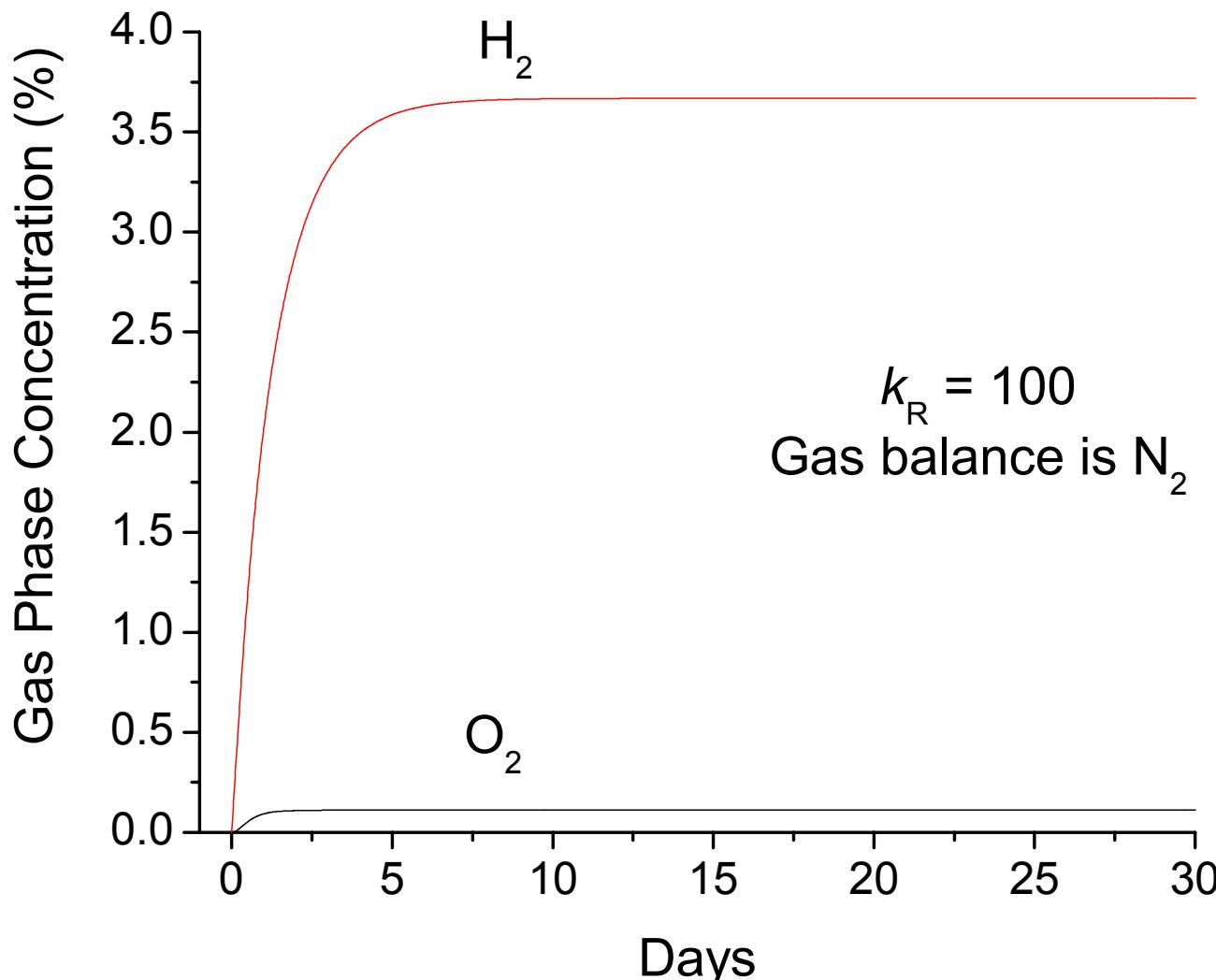


Days

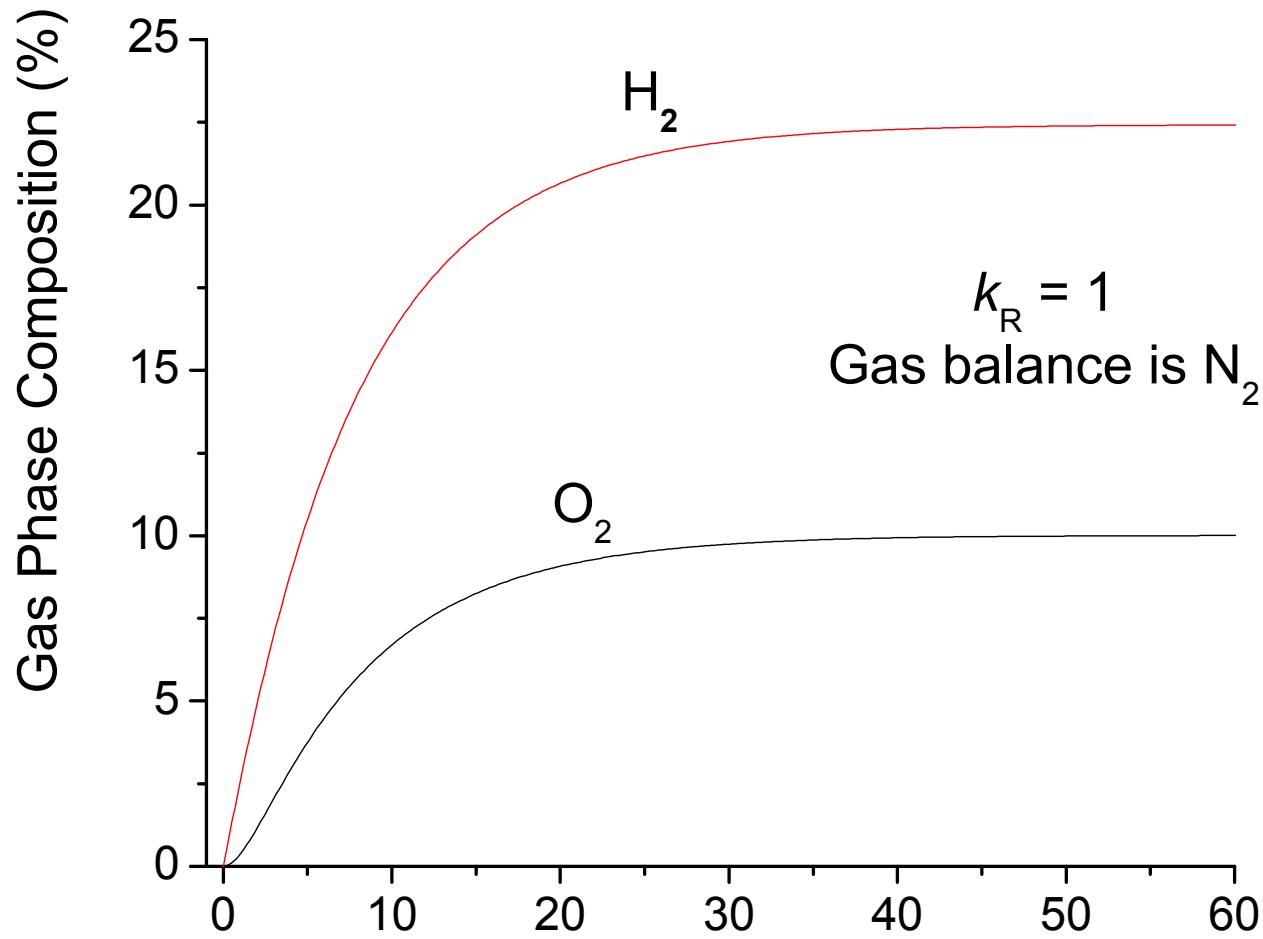
sept6x1



# Gas Phase Composition



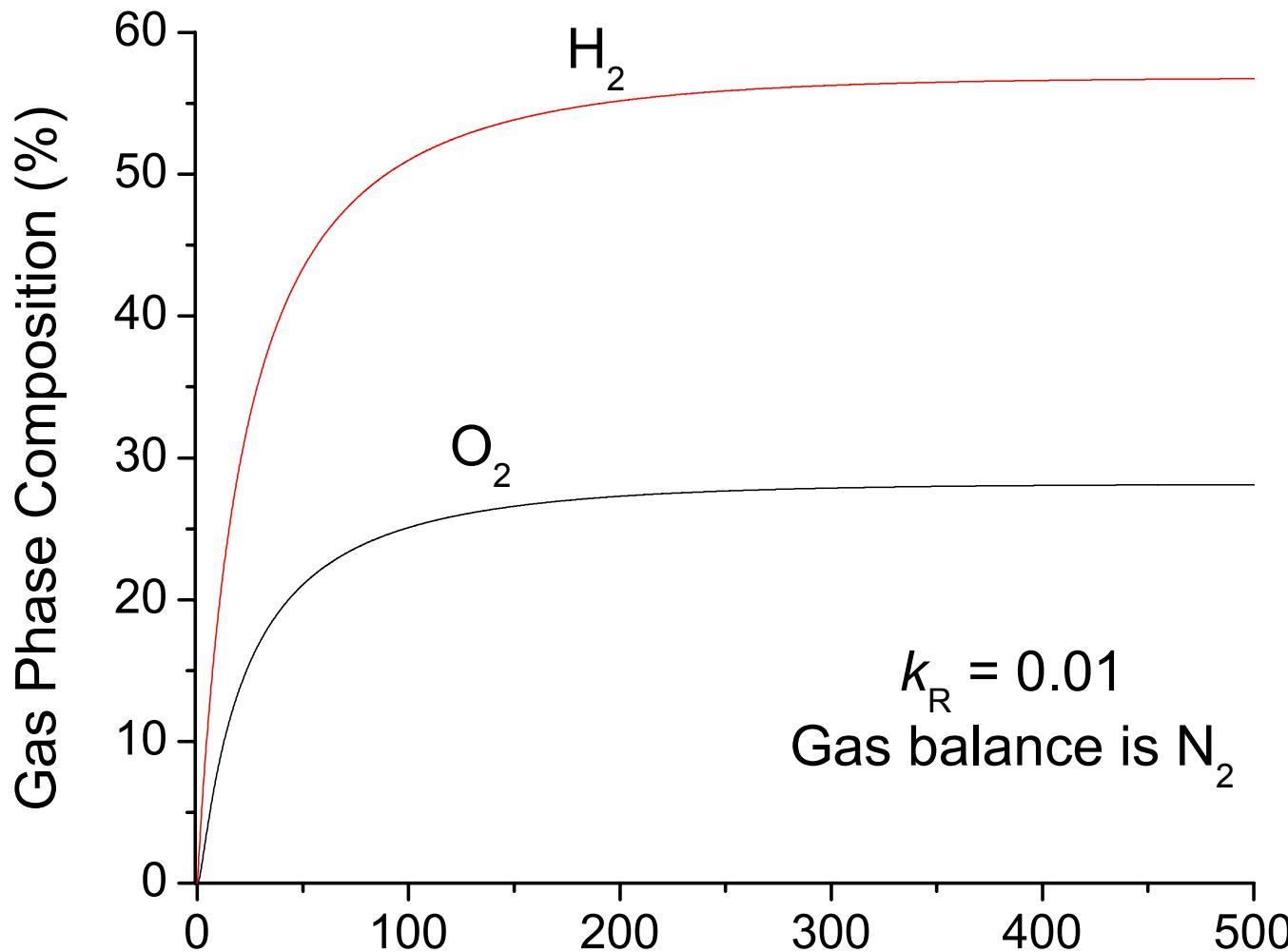
# Gas Phase Composition



Days



# Gas Phase Composition



# Equilibrium Results

$k_R$	Days till equilibrium	Pressure (psia)	% H <sub>2</sub>	% O <sub>2</sub>	% H <sub>2</sub> O still adsorbed
100	10	17	3.7	0.1	99.94
10	12	18	7.6	2.2	99.86
1	50	24	22	10	99.46
0.1	250	49	45	22	97.78
0.01	700	108	57	28	93.89

